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New Calculations of Fe Spectra in High-Temperature Plasmas

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Spectroscopic data acquired during the ASCA performance verification phase have revealed a discrepancy between measured line flux ratios and the predictions of standard plasma emission codes. In plasmas for which coronal ionization equilibrium should apply, flux ratios of 4-2 and 3-2 line complexes in highly-ionized Fe are observed to be significantly lower than predicted, thus compromising the quality of spectral fits. We have recalculated Fe L-shell spectra using the HULLAC atomic physics package and present results for the ionization stages Fe XXI-XXIV. Our preliminary results show (4-2)/(3-2) ratios that are substantially smaller than those tabulated in the commonly used spectral models and point to the possibility of bringing theoretical spectra into accord with the observations.

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CONCLUSIONS

The summed 3-2 (L_{α}) flux in the Fe L-shell ions, as it is incorporated into current spectral fitting packages, is an underestimate at high temperatures. The 4-2 (L_{β}) flux is generally overestimated. The net result is an underestimate of the ratio of the Fe line flux near the 1 keV spectral region to that near the 1.5 keV spectral region.

This result affects determinations of electron temperature, emission measure, charge state distribution, and relative elemental abundances. Revision of Fe atomic data is warranted.

Depending on the observability of Fe line emission and the quality of the data, reliability of interpretations of ASCA data may be compromised.

For the future:

Cascades following dielectronic recombination can contribute significantly to the total line flux by way of *thousands of individually unobservable* lines. Ironically, this is a somewhat ignorable problem with high-resolution spectroscopy, where DR-driven line complexes are partially observable, but crucial for low-to-moderate resolution data, where these lines add (seemingly) inconspicuously to the spectral "bumps".

Calculations underway for the remaining Fe L-shell ions Fe XVII-XX (Liedahl, Osterheld, & Goldstein).

Comparable data being prepared for case of photoionized plasmas, which is relevant to line formation in X-ray binaries and active galactic nuclei (Liedahl, Kahn, Osterheld, & Goldstein).

Experimental program to calibrate Fe L-shell emission to begin this year using an Electron Beam Ion Trap (EBIT) (Beiersdorfer, Kahn, Savin, & Liedahl).

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SUMMARY

Statement of the Problem: ASCA spectra show deviations from predictions of standard plasma emission codes [MEKA (extension of Mewe, Gronenschild, & van den Oord 1985), RAYMOND (based on Raymond & Smith 1977)]. These codes apparently overpredict the line flux near 1.5 keV and/or underpredict the line flux near 1 keV.

Possible Solution: Fe line complexes from 3-2 (~ 1 keV) and 4-2 (~ 1.5 keV) transitions of high ionization states (Fe XXI-XXIV) provide the dominant line flux at high temperatures ($T > 10^7$ K). New calculations of Fe L-shell spectra show reduced (4-2)/(3-2) ratios relative to current models. Specifically, the new calculations show that, for $kT > 1.2$ keV, the 3-2 flux should be *increased*, while the 4-2 flux should be *decreased*, relative to the existing atomic models.

Calculations: Line intensities are computed by solving for the level populations in each ion at a given temperature and density. Atomic data -- level structure, radiative rates, collisional rates -- are calculated using HULLAC, a collisional-radiative atomic modeling package. Models consist of configurations $1s^2(2s2p)^k$, $1s^2(2s2p)^{k-1}3l$, and $1s^2(2s2p)^{k-1}4l$, along with all relevant collisional rates and radiative decay rates. To compare directly with the MEKA code, we use the Arnaud & Rothenflug (1985) Fe charge state distribution.

Application: The results apply to any high-temperature plasma in which the line emission is driven primarily by electron impact excitation -- stellar coronae, supernova remnants, and galaxy clusters.

Figure 1

Figure 2: Some degree of approximation expedites the use of plasma emission codes. For example, lines are often “lumped” together. This does not seriously affect the analysis of low-to-moderate resolution spectra, provided that the total fluxes and the energy centroids are accurate. Here we compare the spectra of three Fe ions, as predicted by MEKA and HULLAC, plotted at “high” resolution $\Delta\lambda = 0.05 \text{ \AA}$. Note the large discrepancy in the *details* of the spectra, particularly below $10 \text{ \AA}$.

Figure 3: The models shown in Figure 2, after folding through a sliding gaussian resolution kernel similar to the ASCA SIS.

Figure 4: Fe XXIV Line Power vs. Temperature

Figure 5: Fe XXIII Line Power vs. Temperature

(Line Power)/(10^{-25} erg cm 3 s $^{-1}$)

Figure 7: Fe XXI Line Power vs. Temperature

(Line Power)/(10^{-25} erg cm 3 s $^{-1}$)

Figure 6: Fe XXII Line Power vs. Temperature

Figure 8: Total Fe Line Power vs. Temperature

Figure 8: Combining the results of Figures 4-8 yields the total Fe line power over the T range 1-2 keV. MEKA underestimates 3-2 flux, relative to HULLAC, by factor ~ 1.7 . The 4-2 fluxes are not as discrepant. Downturn of the MEKA 4-2 curve moving to low temperatures results from omission of Fe XXI 4-2 lines from MEKA code.

Figure 9: (3-2)/(4-2) ratios of Fe line complexes

Figure 9: The observable consequences can be summarized by plotting the ratio $P(3-2)/P(4-2)$, where P denotes the total line power summed over all Fe ions and soft X-ray transitions within each complex. The results differ by approximately 17% at $kT = 1$ keV and 55% at 2 keV.

Figure 10: Moving to higher temperatures, the discrepancy worsens. Here, we show an ASCA SIS simulation of a typical coronal source with $kT = 2$ keV. *Top:* MEKA result. *Bottom:* MEKA result modified by new HULLAC Fe L-shell data. The spectra in the figures below include all of the cosmically abundant elements. Of particular importance, the 8-9 Å emission contains Mg XII Ly α (8.42 Å), while Ne X Ly α (12.13 Å) contributes to the 10-13 Å blend. Clearly, the crucial modification is the increase in 3-2 flux, as found in the new calculations.

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